Quantum Monte Carlo simulations of infinitely strongly correlated fermions

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(February 1, 2008)

Abstract

Numerical simulations of the two-dimensional t-J model in the limit $J/t \ll 1$ are performed for rather large systems (up to $N = 12 \times 12$) using a world-line loop-algorithm. It is shown that in the one-hole case with $J = 0$, where no minus signs appear, very low temperatures ($\beta t \sim 3000$) are necessary in order to reach Nagaoka's state. $J/t \lesssim 0.05$ leads to the formation of partially polarized systems, whereas $J/t \gtrsim 0.05$ corresponds to minimal spin. The two-hole case shows enhanced total spin up to the lowest attainable temperatures ($\beta t = 150$).

PACS numbers: 75.10.Jm

Since the discovery of high-T_c superconductors (HTS), a great deal of interest was focused on strongly correlated systems like the Hubbard and t-J models. Especially the latter system attracts a lot of attention since it can be viewed as a model on its own right for HTS [1] and not only as the strong coupling limit of the Hubbard model. A key method for their understanding is provided by numerical simulations. For the Hubbard model, quantum Monte Carlo (QMC) simulations [2] can be performed for not too large values of the interaction U ($\lesssim 12$ in units of the hopping matrix element t) and also not too large inverse temperatures β ($\lesssim 10/t$), except for the half-filled case, where the so-called minus-sign problem is absent, limiting thus our understanding of the doped phase at low temperatures in the strong coupling limit. On the other hand, exact diagonalizations of the t-J model [3] provide information of precisely that limit but confined to rather small sizes N ($\lesssim 30$). QMC simulations for the t-J model were successfully performed in one-dimension [4], whereas previous simulations in higher dimensions suffered under metastability problems [5] or were restricted to the computation of energies in the ground state [6]. Further numerical studies were carried out using high-temperature expansions (HTE) [7,8] and density-matrix renormalization-group (DMRG) [9,10].

In this Letter QMC simulations of the t-J model are presented for the first time for large systems ($N \lesssim 12 \times 12$) and a large temperature range. Large system sizes are necessary especially in the case $J = 0$, as shown by Barbieri et al. [11], where a change in the stability of the fully polarized ferromagnetic state is observed for two holes at around $N = 12 \times 12$. The simulations are based on a recently developed world-line loop-algorithm [12]. We use a representation of the t-J model where it is obvious that it has no minus sign problem in the case of one hole and $J = 0$ [13,14]. As shown below, this enables us to reach very low temperatures ($\beta t \sim 3000$), that are necessary to converge to Nagaoka's ferromagnetic ground state. Such a slow convergence suggests that a high density of low lying excitations is present. We interpret them in the frame of a spin-wave theory, such that an effective ferromagnetic exchange interaction J_{eff} can be assigned for each lattice size. Finite-size scaling shows, that $J_{eff} \to 0$ in the thermodynamic limit as is expected. Hence, Nagaoka's ferromagnetic state has zero spin-stiffness in that limit. A frequently addressed question is the stability of Nagaoka's state for $J \neq 0$ or more than one hole [15–17]. Our simulations show that for $N = 10\times 10$, $J \gtrsim 5\times 10^{-4}$ suffices to bring the system to a ground-state without maximal spin. Due to the minus-sign problem, simulations for more than one-hole could not be performed at temperatures as low as in the one-hole case ($\beta t \lesssim 150$) and less conclusive results could be obtained. However, it should be remarked that such temperatures are by far lower than those reached previously by either QMC ($\beta t \lesssim 2$) [5] or HTE ($\beta t \lesssim 5$) [8]. Finally, on increasing J, we show that the system goes to minimal spin at $J/t \gtrsim 0.05$. At smaller J the system is partially polarized.

We first describe shortly the representation of the t-J model used in the simulations. Exact operator identities lead to a decomposition of the standard creation ($c^\dagger_{i,s}$) and annihilation ($c_{i,s}$)operators for fermions with spin $s = \uparrow, \downarrow$ [13,14]

$$c^\dagger_{i,\uparrow} = \gamma_{i,+} f_i - \gamma_{i,-} f^\dagger_i \,, \quad c^\dagger_{i,\downarrow} = \sigma_{i,-}(f_i + f^\dagger_i) \,, \tag{1}$$

where $\gamma_{i,\pm} = (1 \pm \sigma_{i,z})/2\,,\ \sigma_{i,\pm} = (\sigma_{i,x} \pm i\sigma_{i,y})/2$, the spinless fermion operators fulfill the canonical anticommutation relations $\{f^\dagger_i, f_j\} = \delta_{ij}$, and $\sigma_{i,\alpha}\,,\ \alpha = x, y,$ or z are the Pauli matrices. The constraint to avoid doubly occupied states reduces in this case to

$\sum_i \gamma_{i,-} f_i^\dagger f_i = 0$ which is a holonomic constraint in contrast to the one normally used with the standard representation. Moreover, this constraint commutes with the Hamiltonian (2), such that once the simulation is prepared in that subspace, it remains there in the course of the evolution in imaginary time. The t-J Hamiltonian in this new representation has the following form

$$H_{t-J} = t \sum_{<i,j>} \left(P_{ij} f_i^\dagger f_j + \frac{J}{2} \Delta_{ij} (P_{ij} - 1) \right) , \tag{2}$$

where $P_{ij} = (1 + \vec{\sigma}_i \cdot \vec{\sigma}_j)/2$, $\Delta_{ij} = (1 - n_i - n_j)$, and $n_i = f_i^\dagger f_i$. The constant added in (2) ensures that H_{t-J} reduces to the standard t-J model. In the case of one hole with $J = 0$, there is only one fermion present and the simulation has no minus-sign problem due to the exchange of fermions. For $J > 0$ a minus sign can occur because the exchange of two spins in space time generates them.

Next we describe the world-line loop-algorithm. The world-lines are as usually defined by checkerboarding space-time [18]. However, a direct application of this algorithm in two spatial dimensions is not effective in dealing with identical particles, since each permutation of any two particles represents a different sector that cannot be reached from another one. Especially in the case of fermions, the minus signs would lead to an extremely innacurate estimate of any observable. This difficulty can be overcome with a loop algorithm [12], which does not preserve the linking topology of the world-lines. Since we are dealing with three states per site, two world lines are introduced (one for the fermions and one for the spin-ups) and their updating is performed separately, the sequence being chosen at random. Technical details will be published elsewhere [19].

In the following we describe the results for the limit $J \to 0$ and mainly with one hole. Figure 1 shows the structure form factor

$$S(\vec{q}) = \frac{1}{N} \sum_{\vec{x}_i} \left(exp\,(\imath \vec{x}_i \cdot \vec{q}) \sum_j S_j^z S_{j+\vec{x}_i}^z \right) \tag{3}$$

at $\vec{q} = 0$, i.e. $< {S_{Tot}^z}^2 >$ for $N = 8 \times 8$ and $N = 10 \times 10$ sites, as a function of βt. As can be clearly seen, very low temperatures are needed in order to reach the fully saturated ferromagnet as predicted by Nagaoka's theorem. This suggests that a high density of low energy excitations is present as would be expected in the case of a Heisenberg ferromagnet. As a simple test of this hypothesis, we compare the temperature dependence of $S(\vec{q} = 0)$ from the QMC simulation with a spin-wave result, where the ferromagnetic exchange coupling J_{eff} of the hypothetical Heisenberg ferromagnet is chosen such as to fit the results of the simulation in Fig. 1. Figure 2 shows that $J_{eff} \propto 1/N$, such that in the thermodynamic limit the spin-stiffness vanishes.

Figure 3 shows that, at the attainable temperatures, the ferromagnetic correlations are enhanced by adding a second hole to the system ($N = 12 \times 12$), suggesting a picture of a ferromagnetic polaron surrounding each hole, with a size limited by thermal fluctuations. Our result is consistent with a stability analysis by Barbieri et al. [11], where the Nagaoka state is stable for two holes and $N \gtrsim 12 \times 12$. However, such a comparison should be taken with care since the results of Ref. [11] are strictly valid in the limit $N_h \ll \ln N$, where N_h is the number of holes. Also DMRG studies [10] support a Nagaoka state for such a low

doping ($\delta \sim 1.4\%$), although the geometry used in that case is quite different from ours. Unfortunately, the minus-sign problem precludes simulations at lower temperatures, such that the ground state cannot be reached. In fact, by comparing Fig. 3 with Fig. 1, it is clear that in order to extract conclusions about the total spin in the ground-state, temperatures much lower than $\beta t = 150$ are necessary, such that previous assertions on the character of the ground state from results at $\beta t = 2$ to 5 [5,8] are doubtful.

Exact diagonalization studies have shown, that the Nagaoka state breaks down for $J > J_1 \sim 0.075t$ in a 4×4 system [20]. Further they show, that the system goes to minimal spin at $J_2 \gtrsim 0.088$. Between J_1 and J_2 the system is partially polarized. In the following we show, that for larger systems ($N = 10 \times 10$) J_1 and J_2 are of different order of magnitude. Whereas Fig. 4 shows that the system is partially polarized for $J = 0.0005t$, Fig. 5 demonstrates that for $J \gtrsim 0.05t$ the system goes to a state with minimal total spin. At the same time, antiferromagnetic correlations begin to dominate at low temperatures. Although the minus sign problem does not allow a very accurate determination, our data show, that the system is partially polarized for $0.0005 \lesssim J \lesssim 0.05$. The last boundary is somewhat higher than the lower bound proposed for the Hubbard-model to reach an antiferromagnetic state in the one-hole case ($U_c^{AF} > (4t/\pi) N \ln N$) [21].

Summarizing, we have performed QMC simulations of fermions in the limit of infinitely strong correlations. The world-line loop-algorithm allows simulations of rather large systems ($N \lesssim 12 \times 12$) and very low temperatures (up to $\beta t \sim 3000$). Such temperatures are necessary in order to reach the fully polarized state in the case of one-hole and $J = 0$. $J/t \lesssim 0.05$ leads to the formation of partially polarized systems, whereas $J/t \gtrsim 0.05$ corresponds to minimal spin. The two-hole case shows enhanced total spin up to the lowest attainable temperatures ($\beta t = 150$).

We are very gratefull to Antimo Angelucci for instructive discussions on the initial stages of the project. The calculations were performed at LRZ München and HLR-Stuttgart. We thank the above institutions for their support.

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FIGURES

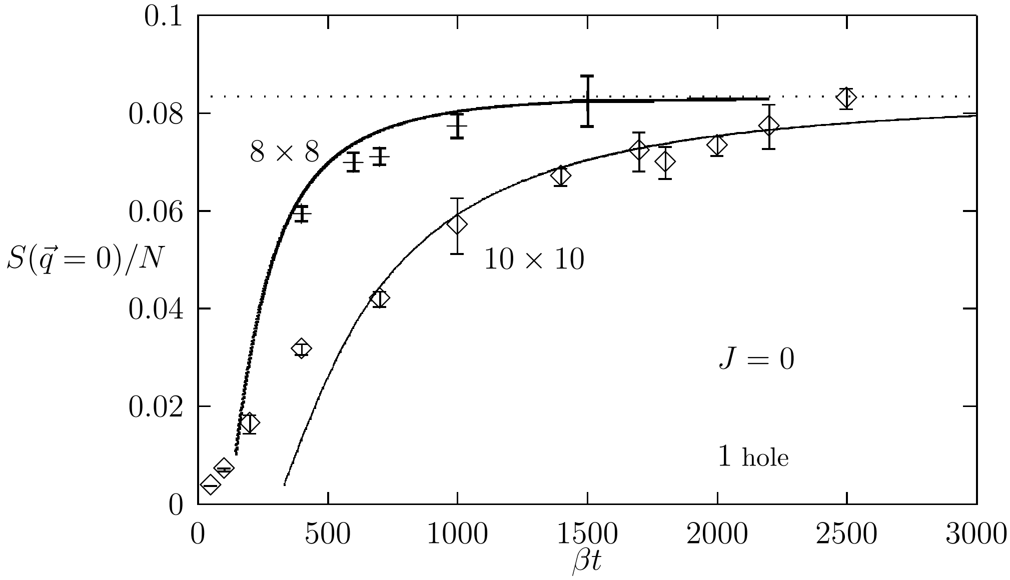
FIG. 1. $S(\vec{q}=0)/N$ for $N = 8 \times 8$ and 10×10, with one hole at $J = 0$. The dotted line represents the fully saturated ground state. The full lines correspond to $S(\vec{q}=0)$ of a Heisenberg ferromagnet in spin wave theory with $J = 0.0065t$ and $J = 0.0030t$, respectively.

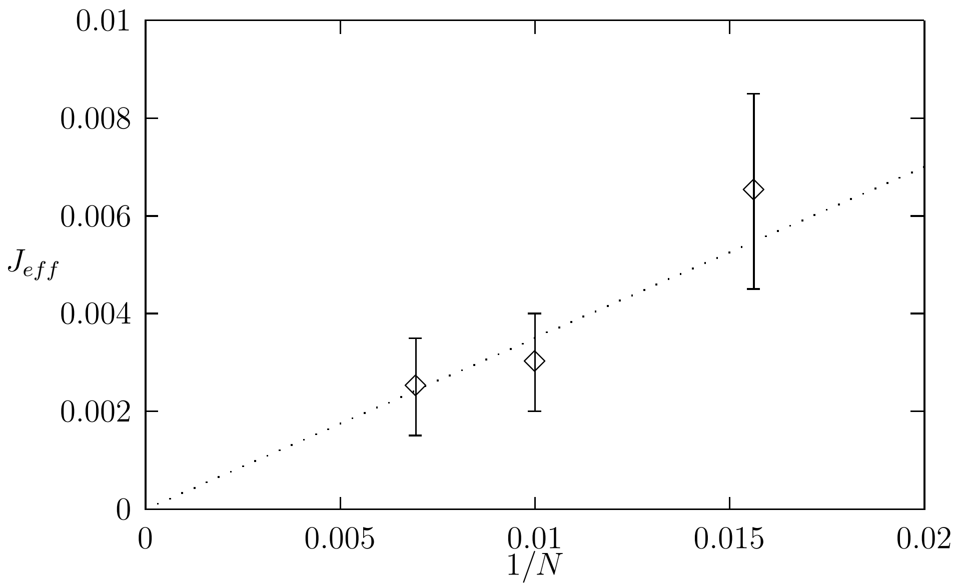
FIG. 2. J_{eff} of the Nagaoka state for different lattice sizes N.

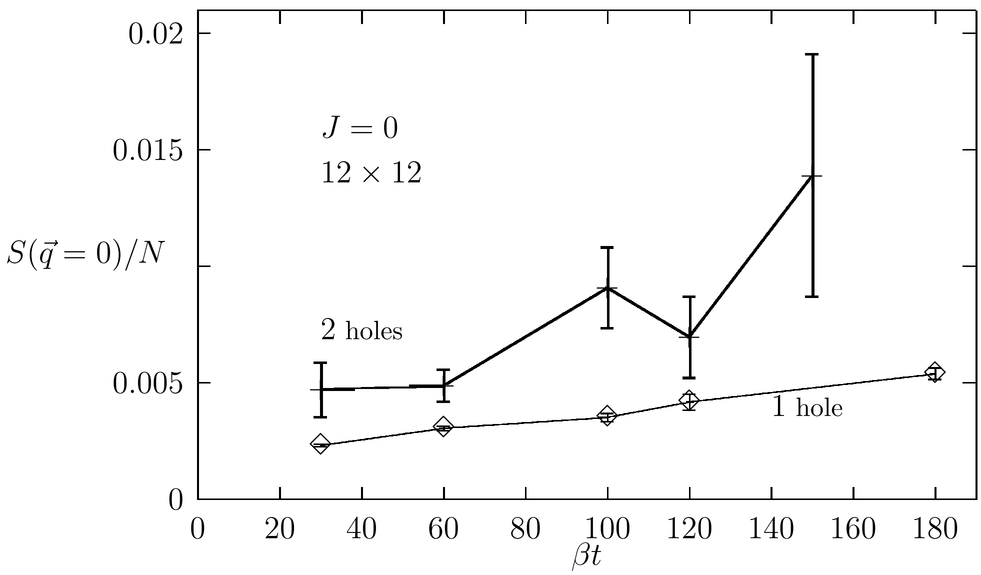
FIG. 3. Comparison of one hole and two holes in a 12×12 lattice. One sees, that ferromagnetism is enhanced by adding another hole.

FIG. 4. $S(\vec{q}=0)$ for a 10×10 lattice with one hole at $t \gg J > 0$.

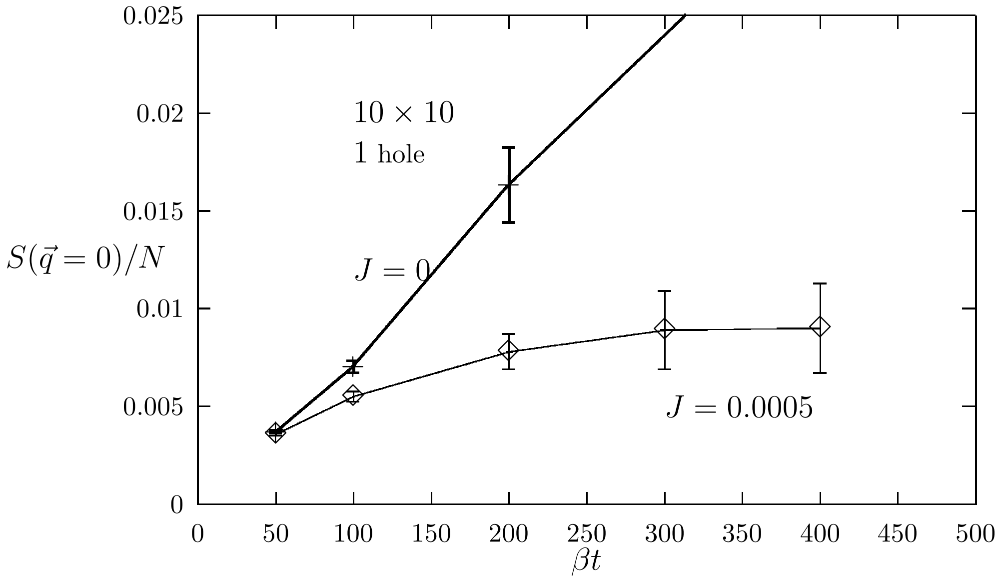
FIG. 5. $S(\vec{q})$ for $\vec{q}=0$ and $\vec{q}=(\pi,\pi)$ for a 10×10 lattice with one hole at $J = 0.05t$


0.1
0.08
0.06
0.04
0.02
0
$S(\vec{q}=0)/N$
8×8
10×10
$J = 0$
1 hole
0
500
1000
1500
2000
2500
3000
βt

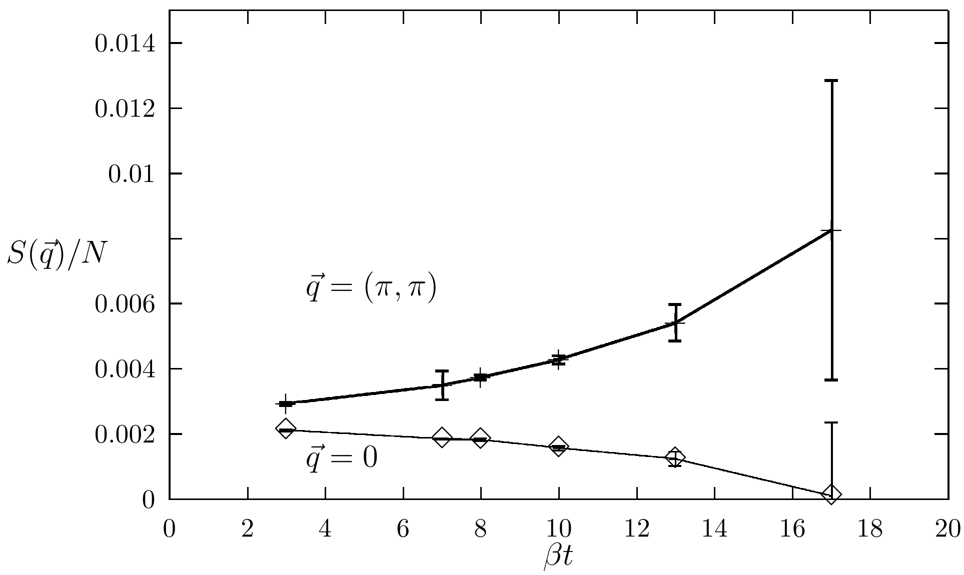

0.01
0.008
0.006
0.004
0.002
0
J_{eff}
0
0.005
0.01
0.015
0.02
$1/N$



0.02
0.015
0.005
0
$S(\vec{q}=0)/N$
$J=0$
12×12
2 holes
1 hole
0
20
40
60
80
100
120
140
160
180
βt



10×10
1 hole
$J = 0$
$J = 0.0005$
$S(\vec{q}=0)/N$
βt
0.025
0.02
0.015
0.01
0.005
0
0
50
100
150
200
250
300
350
400
450
500


0.014
0.012
0.01
0.006
0.004
0.002
0
$S(\vec{q})/N$
$\vec{q} = (\pi, \pi)$
$\vec{q} = 0$
0
2
4
6
8
10
12
14
16
18
20
βt